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DEVELOPMENT OF MULTISCALE APPROACH TO MODELING MECHANICAL RESPONSE OF HIGH-STRENGTH INTERMETALLIC ALLOYS ON THE BASIS OF MOVABLE CELLULAR AUTOMATON METHOD

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Summary. On the basis of movable cellular automaton method (MCA) was developed a multiscale two-dimensional structural and rheological model of hard-strength intermetallic alloy Ni_3Al. In this model, the intermetallic alloy is regarded as multiscale composite system. Developed approach takes into account the properties of grain boundaries, the characteristics of the geometry and internal structure of the grains and their size distribution. Internal grain structure of hard-strength alloy is constructed in the framework of MCA method using the algorithm of Voronoi tessellation. To simulate the processes of deformation and fracture of such complex systems by MCA method the two-dimensional model of elastic-plastic interaction of cellular automata is used. This model is based on the use of many-particle potentials/forces of interaction of cellular automata. An incremental theory of plasticity of isotropic medium with von Mises plasticity criterion was used to model deformation of intermetallic alloy. Radial return algorithm of Wilkins was adopted for this purpose. Two-parameter criterion of Drucker-Prager was used as fracture criterion in proposed model. When modeling of the mechanical response of hard-strength alloy peculiarities of its multiscale internal structure (the presence of subgrains in grains) at lower scales with respect to the considered one was taken into account implicitly using a specially developed multiscale approach. Verification of the developed model is performed by simulation of tests on the uniaxial tension of Ni_3Al samples and comparing the simulation results with the experimental data. Comparison of the obtained "theoretical" loading diagrams with experimental data showed good qualitative and quantitative similarity. This indicates the adequacy of the developed model and the possibility of its use to describe the deformation and fracture of such complex heterogeneous systems.

1 INTRODUCTION

Perspective materials for modern tribological systems are alloys based on the intermetallic compound Ni_3Al, which is characterized by a high melting point, low density, high values of

the heat resistance and corrosion resistance. Increase of strength and durability of the intermetallic alloy under above conditions is possible by grinding of their grain structure by severe plastic deformation of the intermetallic compound in a narrow time interval of its existence in the combustion wave of a powder mixture of nickel-aluminum stoichiometric composition (i.e., in the SHS process). Results of experiments showed that the plastic deformation of the product of high temperature synthesis leads to the formation in the intermetallic compound Ni_3Al of the multiscale grain structure that contains multigrain (grains consisting of subgrains of submicron dimension). This leads to multiple increase in strain to failure limit, strength and other operating characteristics of such intermetallic alloy [1,2]. The reasons for a significant increase in the mechanical properties of high-strength alloy are still uninvestigated in detail. Obtaining of this information is possible only within the framework of an integrated multidisciplinary approach at the intersection of materials science, chemical kinetics, solid mechanics and advanced computational methods. For the implementation of computer simulations of the mechanical response of such complex heterogeneous materials it is necessary to use a multiscale approach, taking into account the mechanisms of deformation and fracture at different scales. In this regard, this paper is devoted to the development of structural and rheological model for the investigations of regularities of the mechanical response of Ni_3Al alloy with multimodal internal structure under extreme loading conditions. This model is developed in the framework of a representative of particle method - method of movable cellular automata (MCA) [3-5].

2 MODEL DESCRIPTION AND ITS VERIFICATION

A two-dimensional structural model of intermetallic Ni_3Al was developed in the paper. In tha framework of this model each grain of material is simulated by an ensemble of movable cellular automata with appropriate rheological parameters (thus, the cellular automaton simulates some fragment of a grain). Fig. 1 shows a schematic structure of an idealized sample of the intermetallic Ni3Al, consisting of grains of complex geometric shapes. This structure was obtained using a specially developed algorithm of Voronoi tessellation [6].

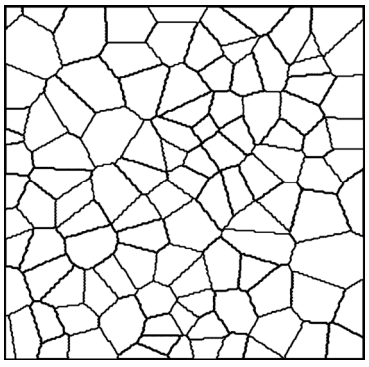

Figure 1. Schematic representation of a fragment of the model structure of the intermetallic alloy obtained using the algorithm of Voronoi tessellation.

On this example, the model sample size is 300×300 microns. Presented sample consists of

110 grains whose average size is 32 microns. Fig. 2 shows the grain size distribution in the model sample. It can be seen that size of most of the grains is in a narrow range of 25 to 40 microns, which corresponds to the grain size distribution in real material.

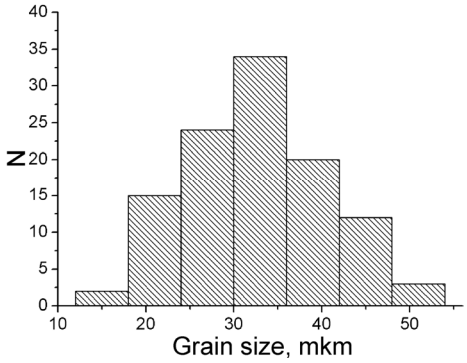

Figure. 2. The distribution of grain size in the model sample.

To simulate the processes of deformation and fracture of such complex systems by MCA method the two-dimensional model of elastic-plastic interaction of cellular automata is used [3-5]. This model is based on the use of many-particle potentials/forces of interaction of discrete elements (cellular automata). The general expression for the element interaction force involves a pair-wise and a volume-dependent part. A key part of the model is a definition of pressure in the volume of a discrete element and its use as a volume-dependent constituent for the force of element interaction with surroundings. A fundamental advantage of the model to building discrete element interaction is concerned with its capability to realize various rheological models of material behavior. In particular, an incremental theory of plasticity of isotropic medium with von Mises plasticity criterion was implemented within the framework of DEM to model deformation of grains on the mesoscopical scale. Radial return algorithm of Wilkins was adopted for this purpose. Capabilities of the developed model makes it possible to describe the mechanical response (including fracture) of elastic-brittle and elastic-plastic isotropic media within approximations of plane stress and plane strain states (in the following calculations the plane stress approximation is used). Elastic constants of the material and the diagram of uniaxial loading are used as input parameters for the model of interaction of cellular automata. These parameters determine mechanical response function of movable cellular automaton (this function is also expressed in terms of "σ–ε" similar to loading diagram).

An important role in building the mechanical model of composites belongs to determining the strength criterion (fracture criterion) and the parameters of the chosen criterion. It is well-known that fracture is a fundamentally brittle and extremely localized phenomenon. Since the physical mechanisms of fracture are concerned with break of interatomic bonds and spatial separation of atomic layers, the criterion for material failure, in contrast to the criterion of plasticity, can not be determined solely by the shear stresses and should take into account the effect of hydrostatic pressure. Therefore a two-parameter criterion of Drucker-Prager was applied as one for interelement bond failure (fracture criterion) in the proposed model. The

following notation of this criterion was used:

$$\sigma_{\text{int}} 0.5(a+1) + \sigma_{mean} 1.5(a-1) > \sigma_c .$$

Here σ_c is a compressive strength of material, $a = \sigma_c / \sigma_t$ is a ratio of compressive strength (σ_c) to tensile strength (σ_t), σ_{int} and σ_{mean} are local values of stress intensity and mean stress. In the framework of discrete element method fracture is realized through a change (switching) in state of the pair of interacting elements from *linked* state (chemically bonded pair resisting to relative compression/tension and shear) to *unlinked* state (two independent particles, only contact interaction including friction is possible). Since fracture is a local process, when applying the criterion to the pair of interacting automata, variables σ_{int} and σ_{mean} are calculated at a contact point of the pair (at a central point of the surface of pair interaction). Parameters σ_c and σ_t therewith correspond to strength of cohesion/adhesion of contiguous material fragments simulated by the pair of interacting automata. A detailed description of the method of calculating fracture criteria for pairs of interacting movable cellular automata is given in [3-5].

As already mentioned in the introduction, the simulation of the mechanical response of such a complex heterogeneous material as hard-strength intermetallic alloy Ni_3Al is necessary to take into account the mechanisms of deformation and fracture at lower scales relative to the considered one. In particular, for the investigated material must be taken into account that the presence of multigrains in the structure. At the same time an explicit account of multimodal internal structure is rather complicated. Experimental data show that the average sizes of the subgrains (grains of which consists multigrain) an order of magnitude smaller than grains in coarse grain materials. In this regard, an explicit account of the presence of multigrains in the material structure requires considerable decrease of the size of cellular automata, and as a result, a significant increase in computation time. Also becomes more complicated the procedure for setting intergrain interaction within the established model. An alternative to the explicit simulation of multimodal structure is a multiscale simulation procedure which consists of several stages. In the first stage is determined the response function of multigrains by simulation of tests on uniaxial compression and tension of small samples which are simulating fragment of multigrain. In this paper, these samples had a size of 40×40 microns and consisted of grains with an average size 2 microns (the size of a cellular automaton 0.15 microns). The internal structure of these samples is also built using an algorithm of the Voronoi tessellation, as shown in figure 1. To simulate the elastic-plastic subgrains in the intermetallic alloy Ni_3Al the parameters of mechanical response of movable cellular automaton conforming to the mechanical properties of single crystals of the intermetallic. The response function of automaton modeling subgrains is a "σ–ε" elastic-plastic diagram with a linear hardening. This diagram was obtained by approximation of the experimental diagrams for uniaxially compressed macroscopical samples of single crystals of the alloy.

At the second stage of the procedure of multiscale modeling is determined the response function of multigrain with the implicit account of its internal structure. For this is also carried out simulation of tests on the uniaxial compression and tension of the specimens simulating a fragment of multigrain. Their internal structure is not explicitly defined, and each movable

cellular automaton in the sample simulates one subgrain. In these calculations, the sample size is also equal to 40×40 microns, the size of the movable cellular automata is equal to 2 microns. In this case, the response function of such a "homogeneous material" is chosen so that the results of its test on the uniaxial compression and tension loading correspond to diagrams obtained for a multigrain with explicit account of the internal structure at the first stage of multiscale procedure.

Thus, the result of the above procedure is to obtain the response function of multigrains, which later will be used in the calculations for samples of coarse grains alloy. Furthermore, this response function will be set to an arbitrary set of grains (modeling multigrain), which volume fraction in coarse-grained material is determined by the experimental data. So for the simulation of coarse grain hard-strength intermetallic alloy (sample size 300×300 microns, size of movable cellular automaton 2 microns) for a particular set of grains simulating multigrain the response function resulting from the above procedure is used. For the rest of the grains, with no subgrain structure, parameters of the mechanical response function of cellular automata correspond to the mechanical properties of macroscopical samples of the Ni3Al.

It should be noted that the mechanical properties of the obtained material as well as the individual grains/multigrains largely determined by the characteristics of the initial powder mixture (pre-compaction quality, cleanliness, and the width of dispersion of the size distribution of the initial powder components) which may often be less than ideal. The consequence is a inhomogeneity of the distribution mechanical properties in the bulk of the material as well as within individual multigrains. In the paper this feature was taken into account by the introduction of a random deviation of set parameters of the response function (the yield stress, strength and deformation characteristics) for individual grains of the intermetallic alloy around the mean value (the maximum value of the variation in work was 20% of the mean). Note, that this deviations introduced as well as for the coarse grain material, and at all stages of the procedure of the multiscale modeling of the multigrains.

Existing experimental data show that at the grain/subgrain boundaries of Ni_3Al alloy are present particles of the aluminum oxide which leads to embrittlement of the grain interfaces compared with the structural elements (grains/subgrains) themselves. Simulation of this effect in the paper carried out by modifying inter-automata interaction during plastic deformation for the grain boundaries. In the framework of the MCA is modeled by introducing additional conditions to the model of Wilkins, limiting the value of stresses drop. Analysis of the results of microscopic investigations of samples of the SHS intermetallic alloy shows that fracture is fragile and has mainly grain boundary nature. This effect relates to the presence of particles of aluminum oxide (Al_2O_3) at the grain boundaries, whose strength characteristics for compression and tension differ by more than 15 times. At the same time tensile strength of corundum is below and compression one significantly higher than the corresponding parameters of Ni_3Al grain. This effect was taken into account by the assignment of corresponding parameters of fracture criterion for grains and grain boundaries.

For verification of developed structural and rheological model uniaxial tension test of the specimens of the intermetallic alloy Ni_3Al was simulated. Comparison of the obtained loading diagrams with the experimental data (fig. 3) for samples containing 12 vol. % of multigrains

shows that they are in good qualitative and quantitative similarities. Note, that fracture of the model samples has mainly grain-boundary character. This shows the adequacy of the developed structural and rheological model and its prospects for the investigation of deformation and fracture of complex, heterogeneous alloys based on the intermetallic Ni3Al obtained in the process of self-propagating high-temperature synthesis.

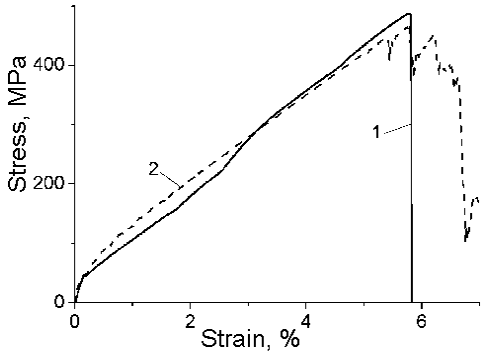

Figure. 3. Loading diagrams (uniaxial tension test) of intermetallic Ni_3Al with 12 vol. % of multigrains: 1 – experimental data, 2 – simulations result.

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